

THE EFFECT OF AN ELECTRIC FIELD OF STRENGTH $-1/2aF^2$ ON THE POLARIZABILITY CONSTANT OF THE NORMAL HYDROGEN ATOM*

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ABSTRACT. Using the integral for the upper limit of the energy in its lowest state of a system as $\int \psi^* H \psi d\tau$ and applying the variation method along the z axis gives the energy. With a field strength of $-1/2aF^2$, produces a negative polarizability constant for the normal hydrogen atom. The value obtained is $a = -58047 \times 10^{-24} \text{ cm.}^3$ which is in close agreement with that obtained by the second-order perturbation theory.

The electric moment of the induced dipole (charge \times distance) is aF , where 'a' is called the 'polarizability' of the atom or ion and F is the strength of the field. Using the integral for the upper limit of the energy in its lowest state of a system as

$$^1E = \int \psi^* H \psi d\tau \quad \dots (1)$$

where H is the complete Hamiltonian operator and is expressed as follows

$$H = T(q, p) + V(q) \text{ and } P = \frac{h}{2\pi i} \frac{\partial}{\partial q}.$$

For the normal hydrogen atom is, with $n=1$, $L=0$, $m=0$ is given by the wave function

$$\psi_{1s} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \quad \dots (2)$$

Using the variation method along the z -axis and multiplying eq. (2) by $(1 + Az)$,

$$\text{Letting } \phi = (1 + Az)\psi_{1s} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} (1 + Az) \quad \dots (3)$$

where $z = r \cos \theta$

The Hamiltonian operator will be in this case

$$H = -\frac{h^2}{8\pi^2} \sum_{m_i} \nabla_i^2 + V \text{ and } V = -\frac{e^2}{r} + e.F.z.$$

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Using H on equation 3 gives

$$\begin{aligned} H\phi &= -\frac{h^2}{8\pi^2} \sum \frac{1}{m_i} \nabla_i^2 \phi + V\phi \\ H\phi &= -\frac{h^2}{8\pi^2} \left(\frac{1}{m_1} \nabla_1^2 \phi + \frac{1}{m_2} \nabla_2^2 \phi \right) + V\phi \\ H\phi &= -\frac{h^2}{8\pi^2} \left(\frac{1}{\mu} \nabla^2 \phi \right) \quad \text{where } \mu = \frac{m_1 m_2}{m_1 + m_2} \\ &= -\frac{h^2}{8\pi^2} \left[\frac{1}{r^2} \cdot \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin^2 \theta} \cdot \frac{\partial^2}{\partial \theta^2} \right. \\ &\quad \left. + \frac{1}{r^2 \sin \theta} \cdot \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) \right] - \frac{e^2}{r} + cFr \cos \theta. \end{aligned}$$

When we substitute $H\phi$ and ϕ in eq. (1) and evaluate over all space, eq. (1) reduces to

$$\begin{aligned} E &= \int_0^{2\pi} \int_0^\pi \int_0^\infty e^{-2r/a_0} \frac{1}{a_0^{3/2}} (1 + Ar \cos \theta) \left[-\frac{h^2}{8\pi^2 \mu} \cdot \frac{1}{r^2} \left\{ \frac{1}{a_0^2} \left(r^2 + Ar^3 \cos \theta \right) \right. \right. \\ &\quad \left. \left. - \frac{1}{r^2 a_0} (2r + 3r^2 \cos \theta) + \frac{2rA \cos \theta}{r^2} - r^2 \left(\frac{1}{a_0} \right) A \cos \theta \right\} - \frac{2Ar \sin \theta \cos \theta}{r^2 \sin \theta} \right. \\ &\quad \left. - \frac{e^2}{r} (1 + Ar \cos \theta) + cFr \cos \theta (1 + Ar \cos \theta) \right] r^2 \sin \theta dr d\phi. \quad \dots (4) \end{aligned}$$

With the following integrals and their values,

$$\int_0^\pi \sin \theta d\theta = 2, \quad \int_0^\pi \sin \theta \cos \theta d\theta = 0, \quad \int_0^\pi \sin \theta \cos^2 \theta d\theta = 2/3 \text{ and}$$

$$\int_0^\infty \sin \theta \cos^2 \theta d\theta = 0 \quad \text{substituted in eq. (4) gives}$$

$$\begin{aligned} E &= \frac{2}{a_0^3} \int_0^\infty e^{-2r/a_0} \left[-\frac{h^2}{8\pi^2 \mu} \left(\frac{2}{a_0^2} - \frac{4}{a_0 r} \right) - \frac{2e^2}{r} + 2/3 cFr^2 A \right. \\ &\quad \left. - \frac{h^2}{8\pi^2 \mu} \left(\frac{2/3 A^2 r^2}{a_0^2} - \frac{2A^2 r^2}{a_0} - \frac{8A^2}{3} - \frac{2A^2 r}{3a_0} \right) - \frac{2e^2 A^2 r}{3} + \frac{2cFr^2}{3} \right] dr \end{aligned}$$

which reduces to the following, when the integrals of this form

$$\int_0^\infty e^{-2r/a_0} r^n dr = \left(\frac{a_0}{2} \right)^{n+1} \frac{1}{n} \quad \text{are evaluated for values of } n=1, 2, 3 \text{ and } 4.$$

Their values are respectively $\frac{a_0^2}{4}$, $\frac{a_0^3}{4}$, $\frac{3a_0^4}{8}$, $\frac{3a_0^5}{4}$.

Therefore a reduced form of equation (4) is as follows,

$$E = \left[\frac{h^2}{8\pi^2 \mu a_0^3} - \frac{e^2}{a_0} + 2eF A a_0^2 + \frac{h^2 \Lambda^2}{8\pi^2 \mu} - \frac{e^2 \Lambda^2 a_0^2}{2} \right]. \quad \dots (5)$$

Since it is not convenient to normalize ϕ we can divide eq. (1) by

$$\int \phi^* \phi d\tau$$

and E will retain its validity.

Evaluating $\int \phi^* \phi d\tau$ and integrating over all space,

$$\begin{aligned} \int \phi^* \phi d\tau &= \int_0^\pi \int_0^{2\pi} \int_0^\infty \frac{e^{-2r/a_0}}{\pi a_0^3} (1 + r\Lambda \cos \theta)^2 r^2 \sin \theta d\theta d\phi dr \\ &= 2 \int_0^\infty \frac{e^{-2r/a_0}}{a_0^3} r^2 dr + \frac{2}{3} \int_0^\infty \frac{e^{-2r/a_0}}{a_0^3} \Lambda^2 r^4 dr \\ &= (1 + a_0^2 \Lambda^2). \end{aligned} \quad \dots (6)$$

Dividing eq. (5) by eq. (6) and letting $h^2 = 4\pi^2 a_0 \mu e^2$, E has the form

$$E = \frac{1}{1 + a_0^2 \Lambda^2} \left(-\frac{e^2}{2a_0} + 2eF a_0^2 \Lambda \right). \quad \dots (7)$$

Differentiating eq. (7) with respect to Λ and equating it to zero gives the equation

$$-2a_0^3 F \Lambda^2 + e\Lambda + 2Fa_0 = 0. \quad \dots (8)$$

Solving for Λ and omitting $16F^2 a_0^4$, because it is small in comparison to the 'e' term, leaves

$$\Lambda = -\frac{e}{2a_0^3 F}.$$

Substituting this value of Λ in eq. (7) reduces it to the following

$$E = -\frac{4a_0^4 F^2}{4a_0^4 F^2 + e^2} \left(\frac{e^2}{2a_0} \right). \quad \dots (9)$$

Since E is given equal to $-1/2aF^2$, equation (9) gives

$$a = -4a_0^3,$$

and then taking the radius of the orbit in the normal hydrogen atom, referred to the center of mass as ² $a_0 = .5282 \times 10^{-8}$ cm., gives $a = -.58947 \times 10^{-24}$ cm.³

Therefore, such a field strength produces a negative 'a' which shows that the induced dipole is in the opposite direction to the field instead of in the same direction. This value of 'a' obtained here is in close agreement with that obtained by the first- and second-order perturbation theory applied to the Stark effect of the hydrogen atom by Epstein,³ Wentzel,⁴ and Waller.⁵

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